A modified nuclear mass formula with a unified prescription for the shell and pairing corrections

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A modified macroscopic-microscopic nuclear mass formula is presented in which shell and pairing effects are simultaneously evaluated by a procedure similar to Strutinsky method. The coefficients of the macroscopic-microscopic mass formula have been adjusted on 2267 experimental atomic masses extracted from the atomic mass evaluation of 2012 (AME2012). Same as the Weizsäcker-Skyrme (WS) model, the influence of the nuclear deformation on the macroscopic energy as well as the mirror nuclei constraint are taken into account, and for the sake of consistency of the model parameters between the macroscopic and the microscopic parts we approximate the isospin-dependent component of the macroscopic energy to the depth of the Woods-Saxon potential. As a result, the root-mean square (rms) deviation with respect to 2267 measured nuclear masses is 0.493 MeV. Then based on the fitted formula we predict the remaining 988 nuclei from the AME2012 for which the masses are still unknown or not well-known, and calculate the $\alpha-$decay energies of seven chains in the superheavy nuclei region with Z =117 and 118.

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I. INTRODUCTION

The accurate knowledge of nuclear masses is of great importance, since it dramatically confines the development of many other areas, like the determination of fundamental constants, symmetry violations, metrology, stellar evolution, and nucleosynthesis [1–4]. Specifically, for example, in nuclear physics, nuclear mass plays an important role in extracting symmetry energy [5], and investigating the evolution of shell closures [6] as well as the limits of nuclear existence [7, 8]. In addition, direct precise mass measurements of nuclei far away from the $\beta-$stable line are of critical importance in interpreting the origin of about half of the heavy elements in nuclear astrophysics [3, 9]. Precise mass values as reliable nuclear physics inputs, are needed for the nuclei along the rp-process path to compare calculations with observations of the light curve profiles and to extract quantitative information about the stellar environments [10, 11].

Theoretically global nuclear mass calculation with increasing precision is always the pursuing aim over the past decades [12–27], and consequently great improvements have been made. Some reviews on the developments and current status of theoretical nuclear masses formula can be seen from Ref. [1, 28]. Noticeably, in very recent years some novel approaches (or models) have been developed and carried out to reproduce the measured nuclear masses systematically onto a fairly excellent precision, such as the microscopic self-consistent mean-field Hartree-Fock-Bogoliubov (HFB) mass models [19, 20], the finite-range droplet model (FRDM) with a more accurate adjustment (FRDM-2011a) [24], and a newly developed mass formula: Weizsäcker-Skyrme (WS) model [21–23] (which considers many corrections, such as isospin and mass dependence, deformation influence to the macroscopic energy, mirror nuclei constraint, and some residual corrections).

Although the macroscopic-microscopic method is a combination of liquid drop model and shell correction approach, its ease of computation as well as its flexibility to choose the nuclear potential is still of great advantage. Moreover, the various effects of the single-particle orbits can be more directly studied in the shell correction approach, while in the self-consistent mean-field models, a clear-cut picture is sometimes lost because of the complicated self-consistency between the nuclear mean field and the effective interaction [29]. Thus, nowadays, despite the great progress of the self-consistent models, the macroscopic-microscopic method remains in frequent use.

Within the framework of the macroscopic-microscopic method the nuclear binding energy of the ground state is the sum of two terms. The well-known macroscopic term is determined by the liquid drop model (LDM) or its variant versions, which is just able to reproduce the smooth trends of binding energy but not the local fluctuations. Hence besides the smooth trend, a microscopic correction term is taken into account for the local fluctuations of binding energy [30–32].

The most important of these fluctuations stems from the shell effects. A very practical and widely used shell correction method is Strutinsky's prescription. It consists of extracting the averaged part of the nuclear binding energy by means of a smoothed single-particle level density. Therefore extracting the average energy as exactly as possible is the central notation for the calculation of the shell correction. In addition, there exists a conspicuous correlation in nuclear ground states, involving the tendency of like nucleons in time-reversed single-particle states to couple to zero total angular momentum [31], which is the so-called pairing correlation. Their most obvious manifestation lies in the characteristic even-odd effect in binding energies. In most of macroscopic-microscopic models the nuclear pairing correction energy is usually treated by means of empirical expression (i.e. piecewise function defined by even or odd nucleon numbers N, Z), but here we deal with it by pure microscopic BCS method.

In fact, both the shell and pair effects associated closely with the level density near the Fermi surface. Thus one often employs simplified expressions for average pairing energy $\bar{E}_p$ by assuming that the smoothed levels are uniformly distributed with the smoothed level density at the Fermi level. But it does not hold exactly for evaluating the pairing correction [29]. Here, for the calculation of $\bar{E}_p$, we give up the simplifications, and directly employ the smoothed level density determined in the shell correction instead. In our calculation, the pairing correction for a given nucleus is defined as the difference between the pairing energy E_p and an average value $\bar{E}_p$, akin to the treatment of Strutinsky shell correction.

It is known that with fewer adjustable parameters as well as rooting on a more fundamental basis, the range of extrapolations is believed to be wider. Inspired by the spirit of more microscopic treatment and fewer model parameters, the purpose of this work is to fit a new mass formula similar to the form of Ref. [25–27], but in modifying it by considering the deformation and microscopic pairing correction in terms of BCS approach. Meanwhile the connection between macroscopic and microscopic parts is also taken into account in our formula by assuming that the isospin-asymmetric part of the Woods-Saxon potential depth approximates to the value of symmetry energy coefficient.

In section II, we present the formula of binding energy and give the details about simultaneous evaluation of the shell and pairing corrections. Then some numerical strategies and details of the mass fitting are also demonstrated. Finally the results and discussion are analyzed in section III. The summary is given in section IV.

II. A MODIFIED NUCLEAR MASS FORMULA

In the macroscopic-microscopic method, the total energy of a nucleus consists of two parts: the macroscopic energy (liquid drop energy $E_{\rm LDM}$) and the microscopic one ($E_{\rm mic}$). Taking into account the influence of nuclear deformation on the macroscopic energy, the expansion of the nuclear binding energy can be assumed as

$$E(Z,A,\beta_k) = E_{\rm LDM}\prod_{k\geq 2}(1+b_k^2\beta_k^2) + E_{\rm mic}(Z,A,\beta_k) \qquad (1)$$
$$b_k = \left(\frac{k}{2}\right) g_1 A^{1/3} + \left(\frac{k}{2}\right)^2 g_2 A^{-1/3}, \quad k = 2,4,6.$$

A, Z are nuclear mass number, charge number, and β_k are deformation parameters. This parabola approximation to the influence of nuclear deformation on the macroscopic energy is verified in terms of Skyrme energy-density functional together with Thomas-Fermi approximation, and more details can be seen in Ref. [21]. The optimal values of g_1, g_2 are finally determined by the measured nuclear masses.

The liquid drop energy in powers of $A^{1/3}$ and $|I|$ (where $I = (N-Z)/A$) [26] is expressed as

$$E_{\rm LDM} = a_v(1-k_v I^2)A + a_s(1-k_s I^2)A^{\frac{2}{3}} + c_1\frac{2-|I|}{2+|I|A}I^2 A + a_c\frac{Z^2}{A^{\frac{1}{3}}}(1-0.76Z^{-2/3}). \qquad (2)$$

Considering the saturation property of nuclear force the volume energy is given by the first term, with I^2A being the asymmetry energy of the Bethe-Weizsäker mass formula [12, 33, 34]. The second term is the surface energy, which accounts for the deficit of binding energy of nucleons at the surface. The third term combined with I^2A dependence of the first two terms consists of the symmetry energy coefficient $a_v k_v + a_s k_s/A^{1/3} + c_1(2-|I|)/(2+|I|A)$. Due to the Coulomb repulsion between protons and diffuseness correction to the sharp radius Coulomb energy (called also the proton form-factor correction in Ref. [12]), the fourth term is included. The detailed evaluations of $E_{\rm mic}$ are presented in the following section.

A. Single-particle potential in microscopic part

The first step in the calculation of microscopic correction is to take a single-particle Hamiltonian. A regular routine is to diagonalize the Hamiltonian in axially deformed harmonic oscillator bases. In order to achieve the diagonalization, we execute a computer code WSBETA [35]. The single-particle Hamiltonian in the program is written as

$$H = T + V + V_{\rm so}, \qquad (3)$$

with the spin-orbit potential

$$V_{\rm so} = \lambda\left(\frac{\hbar}{2Mc}\right)^2 \times \nabla V\cdot(\vec{\sigma}\times\vec{p}), \qquad (4)$$

where λ denotes the strength of the spin-orbit potential, and taking into account the isospin-dependence there are some modifications, i.e. for neutron $\lambda = \lambda_0(1+N/A)$ and for proton $\lambda = \lambda_0(1+Z/A)$. The Woods-Saxon potential takes the form of

$$V = \frac{V_{\rm depth}}{1+\exp\left(\frac{r-R}{a}\right)}, \qquad (5)$$

where a is the diffuseness parameter of the central potential, and R denotes the distance from the point $\boldsymbol{r}$ to the nuclear surface. And the depth of the central potential $V_{\rm depth}$ can be expressed as

$$V_{\rm depth} = V_0 \pm V_s I \qquad (6)$$

with the plus sign for neutrons and the minus sign for protons. V_s is the isospin-asymmetry part of the potential depth. In order to reduce the credibility of extrapolations in the macro-microscopic approach, we assume that V_s approximates to

$a_{\rm sym}$, which bridges up the relationship between the macroscopic and microscopic parts. In this work the relation can be specified as

$$V_s \approx -a_{\rm sym} = -\left(a_\nu k_\nu + a_s k_s/A^{1/3} + c_1 \frac{2-|I|}{2+|I|A}\right), \quad (7)$$

and the values of a_ν, k_ν, a_s, k_s, c_1 are the same as those in Eq.(2).

B. Simultaneous calculation of the shell and pairing correction

The standard Strutinsky shell correction starts from the Dirac generalized single-particle level density (SPLD)

$$g(\varepsilon) = \sum_{i=1}^{M} d_i \delta(\varepsilon - \varepsilon_i), \quad (8)$$

where ε_i, d_i are single-particle energy and its degeneracy respectively, and M is the number of the single-particle levels. Then in terms of convolution the corresponding smoothed SPLD is

$$\bar{g}(\varepsilon) = \frac{1}{\gamma}\sum_{i=1}^{M} d_i K\left(\frac{\varepsilon - \varepsilon_i}{\gamma}\right), \quad (9)$$

where the function $K(x)$ is a bell-shaped kernel one to smear out an arbitrary oscillatory function. In standard Strutinsky method the $K(x)$ often takes the Gauss-Hermit polynomials with the order $p = 6$. The smoothing width $\gamma = 1.2\hbar\omega_0$, and $\hbar\omega_0 = 41A^{-1/3}$ MeV which is the mean distance between the gross shell. Since the shell spacings are $\hbar\omega_0$, the shell corrections are calculated only when $\gamma > \hbar\omega_0$; otherwise, the effect of shells can be noticed in the smooth SPLD [36].

For the pairing correction we consider the simplest seniority-type pairing force and assume the pairing interaction $V_{\rm pair}$:

$$V_{\rm pair} = -G a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j. \quad (10)$$

$\bar{k}$ (for $k = i, j$) represents the label for the time-reversal partner of the $k-$th eigenstate of the single-particle Hamiltonian. It holds that $\epsilon_{\bar{k}} = \epsilon_k$. G is the pairing force strength.

Regardless of quantum SPLD [Dirac $\delta-$type, i.e. Eq.(8)] or smoothed SPLD we take a general form $g(\epsilon)$ and perform the BCS treatment. Therefore the energy of the BCS method can be written as [29, 37]

$$E_{\rm BCS} = 2\int_{-\infty}^{\infty} \epsilon v^2(\epsilon) g(\epsilon) d\epsilon - \frac{\Delta^2}{G}, \quad (11)$$

where the pairing gap Δ is given by

$$\Delta = G\int_{-\infty}^{\infty} u(\epsilon) v(\epsilon) g(\epsilon) d\epsilon. \quad (12)$$

The constraint on the expectation value of the number of particles is expressed as

$$N = 2\int_{-\infty}^{\infty} v^2(\epsilon) g(\epsilon) d\epsilon. \quad (13)$$

where the $u^2(\epsilon)$ and $v^2(\epsilon)$ denote the empty and occupied probability of the single-particle level ϵ, respectively.

By considering only values at discrete points [Eq.(8), $d_i = 2$], i.e. inserting Eq.(8) into Eqs.(11), (12) and (13), we can get the following standard gap equations,

$$\frac{2}{G} = \sum_{i=1}^{M} \frac{1}{\sqrt{(\epsilon_i - \lambda_{\rm BCS})^2 + \Delta^2}}, \quad (14)$$

$$N = \sum_{i=1}^{M}\left[1 - \frac{\epsilon_i - \lambda_{\rm BCS}}{\sqrt{(\epsilon_i - \lambda_{\rm BCS})^2 + \Delta^2}}\right], \quad (15)$$

and the corresponding BCS energy

$$E_{\rm BCS} = \sum_{i=1}^{M}\left(1 - \frac{\epsilon_i - \lambda_{\rm BCS}}{\sqrt{(\epsilon_i - \lambda_{\rm BCS})^2 + \Delta^2}}\right)\epsilon_i - \frac{\Delta^2}{G}, \quad (16)$$

where the pairing gap Δ and the chemical potential $\lambda_{\rm BCS}$ are determined by the two coupled equations for a given force strength G. The pairing energy becomes

$$E_p = E_{\rm BCS} - E_{s.p.} = E_{\rm BCS} - 2\sum_{i=1}^{N_F} \epsilon_i, \quad (17)$$

where $E_{s.p.}$ is the sum of all occupied single-particle level energies, N_F is the number of occupied energy levels. It should be noted that for the last odd nucleon the blocking effects are considered.

The continuous version of the gap equations take form

$$\frac{2}{G} = \frac{1}{2}\int_{-\infty}^{\infty} \frac{1}{\sqrt{(\epsilon - \lambda_{\rm BCS})^2 + \Delta^2}} \bar{g}(\epsilon) d\epsilon, \quad (18)$$

$$N = \frac{1}{2}\int_{-\infty}^{\infty}\left[1 - \frac{\epsilon - \bar{\lambda}_{\rm BCS}}{\sqrt{(\epsilon - \lambda_{\rm BCS})^2 + \Delta^2}}\right]\bar{g}(\epsilon) d\epsilon. \quad (19)$$

By substituting $\bar{\Delta}$ with a value from some empirical formula for the pairing gap, one can determine the Fermi level $\bar{\lambda}_{\rm BCS}$ from Eq.(19) and then the force strength G from Eq.(18). The smoothed BCS energy can be evaluated by

$$\bar{E}_{\rm BCS} = \frac{1}{2}\int_{-\infty}^{\infty}\left[1 - \frac{\epsilon - \bar{\lambda}_{\rm BCS}}{\sqrt{(\epsilon - \lambda_{\rm BCS})^2 + \Delta^2}}\right]\epsilon\bar{g}(\epsilon) d\epsilon - \frac{\bar{\Delta}^2}{G}. \quad (20)$$

Here $\bar{\Delta} = (-12|\frac{N-Z}{A}| + 7.5)/A^{1/3}$ in Ref. [38] is adopted. Similarly the final average value of pairing energy may be written as

$$\bar{E}_p = \bar{E}_{\rm BCS} - \bar{E}_{s.p.}, \quad (21)$$

where $\bar{E}_{s.p.}$ is the smooth of $E_{s.p.}$, which can be obtained by the standard Strutinsky method.

The pairing correction is defined as the difference between the pairing energy E_p of the considered nucleus and that of an averaged value $\bar{E}_p$ for the same nucleus. Let us consider the difference [29, 30]:

$$E_{\rm pair} = E_p - \bar{E}_p, \quad (22)$$

TABLE I: The model parameters of our mass formula. The present rms deviation σ=0.493 MeV, and the average deviation is $\bar{\delta}$ = −0.0108 MeV.

a_v	k_v	a_s	k_s	a_c	c_1	g_1
15.4654	-1.8391	-17.1929	-2.0516	-0.7082	-28.2525	0.0093
g_2	V_0	r_0	a	λ_0	f_1	
-0.4015	-44.9430	1.3880	0.7765	27.8003	0.8557	

then we substitute Eqs.(17) and (21) into Eq.(23) and immediately get

$$\begin{aligned} E_{\rm pair} =&(E_{\rm BCS} - \bar{E}_{\rm BCS}) - (E_{s.p.} - \bar{E}_{s.p.}) \\ =&(E_{\rm BCS} - \bar{E}_{\rm BCS}) - E_{\rm shell}. \end{aligned} \tag{23}$$

As a result the microscopic correction can be casted into

$$\begin{aligned} E_{\rm mic} &= E_{\rm pair} + E_{\rm shell} \\ &= E_{\rm BCS} - \bar{E}_{\rm BCS}. \end{aligned} \tag{24}$$

Taking into account the mirror nuclei constraint and the isospin-symmetry-breaking effect [22], we can further modify the microscopic correction energy by

$$E_{\rm mic} = f_1 E_{\rm mic} + |I| E'_{\rm shell}, \tag{25}$$

where f_1 is a scale factor, because the rms deviation of the fit with the scale factors f_1 can be somewhat reduced. The $E'_{\rm shell}$ is the shell correction energy of mirror nuclei.

C. Numerical details and model parameters

The masses of the 2267 selected nuclei verifying the two conditions: N and Z larger than 7 and the one standard deviation uncertainty on the mass lower than or equal to 150 keV [39] are used.

The macroscopic and microscopic parts of binding energy formula are closely connected by an approximate coefficient $a_{\rm sym}$ of the symmetry energy and other isospin-dependent model parameters. The advantages are that it not only can reduce the number of model parameters, but also can augment the credibility of extrapolations of our mass formula.

Here we have 13 independent adjustable parameters. In the microscopic part, we assume and set the radius and diffuseness of the single-particle potential of protons equal to those of neutrons for simplicity, thus there are only 5 adjustable parameters: V_0 in Eq.(6), diffuseness parameter a, radius parameter r_0, the strength of the spin-orbit potential λ_0, scale factor f_1. In the macroscopic part, there are 8 adjustable parameters: a_v, k_v, a_s, k_s, g_1, g_2, a_c, c_1. These coefficients are obtained by a nonlinear least squares fitting procedure. By varying these adjustable parameters and searching for the minimal deviation of the 2267 nuclear masses from experimental data, we finally obtained the optimal model parameters listed in Table I.

III. RESULTS AND DISCUSSION

The optimal parameters are listed in Table I, and the corresponding rms deviation between the calculated nuclear binding energies and the experimental ones is 0.493 MeV, and the average discrepancy is -0.0108 MeV. Fig. **??**(a) shows the deviations as a function of neutron number. Here the maximal deviation (absolute value) is about 3.72 MeV at $A = 16$ ($N = Z = 8$). In this figure we can also see that the deviations for light nuclei are greatly larger than those for heavy ones, and verify the shortage of LDM in describing the properties of light nuclei, mainly due to the significant structure effect which is much more distinct for light nucleus. For the sake of a statistic understanding of our results, Fig. **??**(b) shows the the statistic behaviors of the deviations from the experimental data. In this figure the solid curve denotes the Gaussian statistic fittings as

$$y = y_0 + \frac{D}{\omega\sqrt{\pi/2}} e^{-2\frac{(x-x_c)^2}{\omega^2}}, \tag{26}$$

where y_0 is the minimum counts, D represents the area of the Gaussian distribution, and x_c and ω denote the statistic averages (ideally zero) and errors. The deviations of binding energies from the data perfectly obey the Gaussian statistic behaviors with $y_0 = 1.98843$, $D = 441.07249$, $x_c = -0.00794$, $\omega = 0.907$. The results of the analysis provide that for 72.21% of nuclei the difference (absolute value) is lower than 0.5 MeV (approximates to σ), and for 99.18% of nuclei the difference (absolute value) is lower than 1.49 MeV (equals to 3σ).

Very recently Sobiczewski *et al.* pointed out that only to supply the rms value of the mass for the global region of nuclei is far from sufficient, because the accuracy of a model strongly depends on the region of nuclei considered [40]. This suggests us to divided the whole region of nuclei under consideration into five subregions [global (all nuclei with $Z, N \geq 8$) (labeled by G), light ($8 \leq Z < 28$) (labeled by L), medium-I ($28 \leq Z < 50$) (labeled by M-I), medium-II ($50 \leq Z < 82$) (labeled by M-II), and heavy ($Z \geq 82$) (labeled by H)]. Then the dependence of the accuracy on this five subregions is illustrated in Fig. **??** with five other models for comparison. One can see that the dependence of the rms on the region of nuclei is very strong, especially for the FRDM, Lublin-Strasbourg drop (LSD) model [41], Hartree-Fock-Bogliubov mean field model with the D1M Gogny interaction (GHFB) [18], and the one carried out by Koura *et al.* (KTUY) [15]. For the four solid line+symbols curves, the trends of the dependence are very similar to each other, i.e. the accuracy of the masses systematically increases when one passes from lighter to heavier nuclei, reflecting the fact that the natures of these macroscopic-microscopic models are very similar (the dashed+symbols showing a different trend denote the accuracy of GHFB and KTUY models which are not macroscopic-microscopic models). Moreover, among all the models the dependence as well as the rms of our formula is relatively the closest one to those of WS3.6 [23].

If only the nuclei verifying $A \geq 50$ are taken into account, i.e. our formula is refitted by a new set of 2051 experimental data, as a result the rms deviation reduces to only 0.437 MeV

for these 2051 nuclei. This might implicit that the assumption of a good mean field on which all the models are based, is better fulfilled for heavier nuclei [40].

It should point out that our formula is very similar to that of WS model in Ref. [22], but there also exist a little difference. In the WS model, the pairing correction simulated by a piecewise function [42], is expressed as

$$\delta_{np} = \begin{cases} 2-|I|, & N \text{ and } Z \text{ even} \\ |I|, & N \text{ and } Z \text{ odd} \\ 1-|I|, & N \text{ even}, Z \text{ odd, and } N > Z \\ 1-|I|, & N \text{ odd}, Z \text{ even, and } N < Z \\ 1, & N \text{ even}, Z \text{ odd, and } N < Z \\ 1, & N \text{ odd}, Z \text{ even, and } N > Z, \end{cases}$$

$$E_{\text{pair}} = a_{\text{pair}} A^{-1/3} \delta_{np}, \tag{27}$$

where Z, N, A and I are proton number, neutron number, mass number and relative neutron excess, respectively. a_{pair} is one of its adjustable model parameters. In our formula the pairing correction is treated in a pure microscopic way as mentioned in Sec.II B, and especially we do not introduce additional adjustable model parameters. To some extent our formula is more concise and microscopic.

In the following we compare our results in several aspects with those of some other models to test our formula and fitting procedure. Firstly, Fig. **??** shows the calculated microscopic corrections of nuclei with our formula [i.e. Eq.(25)] and those obtained by the FRDM. Our results as well as FRDM reproduce the position of the magic number ($N = 20, 28, 50, 82, 126$) and they both give the equivalent magnitude. The deviations are larger for light nuclei and mid-shell nuclei (in the middle of two magic numbers), and our calculations give much larger values (in absolute value) than those of FRDM. For example the microscopic correction of ^{24}O has a value of -8.47 MeV with our formula, while it is 0.32 MeV from FRDM and -4.6 MeV from WS. Experimentally, it is assumed that ^{24}O is a doubly magic nucleus from the observed decay energy spectrum and the high-lying first excited 2^+ state (above 4.7 MeV) [43, 44], which is consistent with our evaluations. It is known that the microscopic energy strongly depends on the single-particle potential employed. Therefore it is the isotopic dependence of the spin-orbit strength and the symmetry potential adopted in our formula that make the microscopic energies different from those of FRDM [21].

The ground state deformation is a very important factor in the description of nuclear mass. A deformed shape weakens the Coulomb energy and enhances the nuclear surface energy relative to a spherical one. In Fig. **??** we show the calculated deformations of each nucleus with our formula for all the 3255 nuclei from Ref. [39]. We obtain the similar results as WS* model [22]. Obviously, the calculated structure of the known magic nuclei is spherical or nearly spherical in shape and the overall amplitudes of β_4, β_6 are indeed relative small versus those of β_2. In addition, for the light nuclei, the β_6 deformations of nuclei are not very obvious, compared to the intermediate and heavy nuclei.

Fig. **??** shows the neutron pairing force strength G_n and the pairing gap Δ_n, and takes Er isotopes chain as an example. In Fig. **??**(a), the neutron pairing force strength G_n determined by Eq.(18) are systematically lower than an empirical trend $G = 20/A$. In Fig. **??**(b) we compare the pairing gap Δ obtained by Eqs.(14) and (15) to empirical trend $\overline{\Delta} = 12/\sqrt{A}$ (dash curve), $\overline{\Delta} = -12|\frac{N-Z}{A}| + 7.5$ (dash dot curve), and the experimental values which are extracted by means of the three-point indicators $\Delta^{(3)}$ [45–47] of the odd-even staggering on nuclear binding energies (OESs). It can be seen that the pairing gap Δ_n calculated by our formula agree well with the experimental OESs. At $N = 82$ the calculated pairing gap $\Delta_n = 0$ is reasonable, since the large shell gap at magic number 82 dramatically depresses the pairing effect. The method which can simultaneously calculate of the shell and pairing correction is reasonable for calculating the microscopic energy.

In addition, in recent decades, the symmetry energy has been one of the hottest topics of nuclear physics owing to its crucial role in understanding a variety of issues in nuclear physics [5**? ? ? ?**].

Mass predictions by using the parameters in Table I (not readjusted) for the remaining 988 nuclei from the AME2012 with $Z, N > 7$ for which the mass is still unknown or known with an uncertainty higher than 150 keV are compared with the extrapolated values in the AME2012 [39]. As a result the rms deviation is 0.847 MeV which is better than 1.35 MeV in Ref. [48] which uses a simplest approach with less adjustable parameters. For about 55% of nuclei the difference is lower than 0.5 MeV and for 81% of nuclei the difference is lower than 1 MeV.

The α emission is one of the decay modes of the heavy nuclei. Measurements on the α decay can provide reliable information on the nuclear structure such as the ground-state energy, the ground-state half-life, the nuclear spin and parity, the nuclear deformation, the nuclear clustering, the shell effects, and the nuclear interaction [49–54]. Theoretically, the precise calculation of the properties of superheavy nuclei could supply important theoretical reference for SHN in experiment. One of the most important applications of the nuclear mass formula is to investigate and predict the properties of superheavy nuclei (SHN), such as the Q-value of $\alpha-$decay and cluster emission. Based on our fitted formula we calculate the $\alpha-$decay energies of seven $\alpha-$decay chains which are isotopes of superheavy nuclei with Z =117 and 118 at the end of the AME2012 masses table. The experimental data of $\alpha-$decay energies are extracted from Ref. [55–57] and references therein. There are 26 experimental data listed in third and seventh columns of Table II. On the whole, we can see from the table that the calculated values agree well with the experimental ones. The rms deviation $\sigma = \sqrt{\sum_i^N [Q_{\alpha,i}(\text{Expt.}) - Q_{\alpha,i}(\text{Cal.})]^2/(N-1)}$ of the $\alpha-$decay energies is 0.6 MeV.

IV. SUMMARY

The coefficients of a modified macroscopic-microscopic nuclear mass formula considering the isospin dependence

TABLE II: The $\alpha-$decay energies Q_α (in MeV) calculated with our formula [Q_α(Cal.)] are compared wit experimental values [Q_α(Expt.)]. The experimental data are taken from Ref. [55–57].

A	Z	Q_α(Expt.)	Q_α(Cal.)	A	Z	Q_α(Expt.)	Q_α(Cal.)
295	118	-	11.81	294	118	11.81(6)	11.95
291	116	10.89(7)	10.77	290	116	11.00(8)	10.86
287	114	10.14(6)	10.08	286	114	10.33(6)	10.46
283	112	9.67(6)	10.75	282	112	-	11.08
279	110	9.84(6)	10.23	278	110	-	10.39
275	108	9.44(7)	9.22	274	108	-	9.31
293	118	-	12.00				
289	116	-	10.96				
285	114	-	10.99				
281	112	-	11.29				
277	110	-	10.56				
273	108	-	9.50				
294	117	10.96(10)	11.26	293	117	11.18(8)	11.40
290	115	10.09(40)	10.01	289	115	10.45(9)	10.10
286	113	9.77(10)	9.97	285	113	9.88(9)	10.52
282	111	9.13(10)	10.47	281	111	-	10.73
278	109	9.69(19)	9.46	277	109	-	9.55
274	107	8.93(10)	8.54	273	107	-	8.65
292	117	-	11.53	291	117	-	11.56
288	115	10.61(6)	10.18	287	115	10.74(9)	10.42
284	113	10.15(6)	11.13	283	113	10.26(9)	11.56
280	111	9.87(6)	10.90	279	111	10.52(16)	11.08
276	109	9.85(6)	9.70	275	109	10.48(9)	9.81
272	107	9.15(6)	8.88	271	107	-	8.76

and microscopic corrections have been determined by an adjustment to 2267 experimental measured masses given in AME2012. For the microscopic correction, without introducing additional parameters, the pairing and shell corrections are simultaneously treated by the Strutinsky prescription.

After a least square fitting procedure for 2267 experimental measured masses, a rms deviation of 0.493 MeV is reached. Moreover, the microscopic corrections and the deformations of every nucleus are also obtained self-consistently in this fitting. From the analysis of the fit results we conclude that: (1) for light nuclei the microscopic corrections in our formula are systematically larger than those from the FRDM model; (2) the deviations of binding energies from the experimental data perfectly obey the Gaussian statistical behaviors; (3) the accuracy of a model depends on the region of nuclei considered; (4) around the known magic nuclei the calculated shapes of them are spherical or nearly spherical, and the overall amplitudes of β_4, β_6 are relative small versus those of β_2.

In addition, if we exclude the $A < 50$ nuclei from 2267 experimental measured ones, i.e. only 2051 experimental data, and refit the parameters, then the rms deviation reduces to only 0.437 MeV for these 2051 nuclei.

Utilizing the optimal parameters listed in Table I we evaluate the neutron pairing force strength G_n's and the pairing gap Δ_n's of Er isotopes as an example. As a results the pairing gap Δ_n's calculated by our formula agree well with the experimental OESs. Finally predictions of the remaining 988 nuclei from the AME2012 with $Z, N > 7$ for which the mass is still unknown or known with an uncertainty higher than 150 keV are compared with the extrapolated values in the AME2012. Moreover, we calculate the $\alpha-$decay energies of seven $\alpha-$decay chains, and the results agree well with the experimental data.

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